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TITLE: Strained-bond semiconductors
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INSTITUTION: Arizona State University

1. SUMMARY

Theories of strained-bond semiconductors and superconductors have been developed that promise to have significant impact on future electronic devices of interest to the Air Force. These include: (a) development of a theory of high-temperature superconductivity based on the idea of strained-layer superlattices, (b) elucidation of the physics of doping in Type-II semiconductor superlattices, which is now central to the development of high-speed field-effect transistors, (c) a theory of dimerization and reconstruction on (001) semiconductor surfaces, (d) theory of Möbius transforms as applied to physics and remote sensing, (e) new understanding of how defects affect the vibrational properties of semiconductors, (f) new methods of efficiently computing the trajectories of atoms in semiconductors by *a priori* molecular dynamics, (g) elucidation of the criteria affecting quantum-well luminescence from Si, (h) models of the effects of vacancies in large-gap $A\ell_xGa_{1-x}N$ alloys, (i) physics of rare-earth-doped silicon, (j) models of Co adsorption to silicon surfaces, (k) theories of how defects affect the properties of large band-gap superlattices, and (l) models of the effects of electronic structure on the properties of semiconductors.

2. OBJECTIVES

Our goal has been to develop theories of semiconductor and superconductor materials that will lead to a better understanding of the physics of these materials, for potential application to devices of interest to the Air Force.

3. STATUS OF RESEARCH

We have made progress on the following problems:

a. Superconductivity

We have developed a theory of high-temperature superconductivity that can explain many data [250,295,308,310,317,318,320,321], and can even predict phase boundaries. Using pair-breaking by rare-earth magnetic impurities as a probe and analyzing voluminous data, we have shown that the superconductivity is rooted in the vicinity of dopant oxygen, not in the cuprate planes (as widely believed), of the high-temperature superconductors. This idea will lead to the overthrow of the leading conventional models, all of which assume that the superconductivity is rooted in the cuprate planes — despite the fact that many high-temperature superconductors exist which have neither layered structures, cuprate planes, nor copper. Hence, our model explains why a successful theory for interpreting data has been so long in coming: everyone has been assuming that the superconductivity originates in the cuprate planes, when in fact it is rooted in the chain layers of materials

such as $YBa_2Cu_3O_x$ with x≈7. Our theory ascribes the superconductivity to oxygen that is under-charged or "neutral" in a sense, and so predicts that there will be entire new classes of high-temperature superconductors. It raises the possibility that superconductors can be integrated with semiconductor devices and operate at reasonable temperatures [310]. The basic idea underlying our model is that the layered high-temperature cuprate superconductors are strained-layer superlattices, whose cuprate planes are under compressive strain, and whose "charge-reservoir" oxygen layers are under tensile strain. The oxygen then can liberate holes which participate in BCS-like superconductivity. Cooper pairs (of holes) are formed *via* the polarization field of the host, which has two main spectral features: a soft-mode (strong-coupling) pairing, and an excitonic ($O^{-2} + 2h^{+} \rightarrow O^{0}$) mode. Both of these are associated with the presence of "neutral" oxygen.

Experiments are under way to test our model, and the preliminary results are all very positive.

b. Type-II superlattices

The physics of defects in Type-II superlattices has been worked out and applied to the $InAs/A\ell_xGa_{1-x}Sb$ [278,279,284,298,307]. We predict that antisite defects that are normally thought of as shallow or deep acceptors can dope the InAs quantum wells of this system n-type! These results are being employed to develop high-speed field-effect transistors by Motorola.

c. Dimerized (001) surfaces

The Si(001) surface dimerizes into long rows of dimers. The GaAs(001) anion-terminated surface prefers rows of about length three dimers. (The cation-terminated surface is predicted to bulge without reconstructing.) We have developed a general theory of (001) semiconductor surfaces which shows that the length of the dimer rows on the anion-terminated surfaces decreases with ionicity. Thus there is competition between the covalent forces, which attempt to make long rows, and ionic forces which attempt to form a $NaC\ell$-like structure on the surface. This is one of the first general theories of semiconductor surface reconstruction.

d. Inverse problems and Möbius transforms

One of the classic problem of physics has been to invert signals detected remotely to determine the nature of the source. (For example, can a plane flying over a field detect the infra-red spectrum radiated from the field and determine if it is coming from a cow or a tank?) We have been at the forefront of the development of Möbius transforms for inverting such problems, and have developed new transforms especially well-suited to physical applications [270].

e. Phonons associated with defects

The theory of lattice vibrations associated with defects in semiconductors is an old field, but we have found some new physics in it, by investigating the normal modes associated with defects. It turns out that some of these modes have remarkable properties, from the viewpoint of basic physics. We are hoping that various experiments will test our

theories [252,255,263].

f. Molecular dynamics

We have developed a new kind of *a priori* molecular dynamics, which has much of the theoretical validity of local density theory, with the computational facility of tight-binding theory [262,271,272]. This method allows us to simulate processes in semiconductors, such as growth, defect migration, and surface relaxation.

g. Silicon quantum-well luminescence

The criteria for developing silicon quantum-well luminescent devices have been developed and clarified [280].

h. Vacancies in $A\ell_xGa_{1-x}N$

The likelihood that visible light-emitters will be preferentially fabricated from III-V nitrides has caused us to examine the role of vacancies in $A\ell_xGa_{1-x}N$. Our theory led to explanation of numerous phenomena [282].

i. Rare-earth doped silicon

We have developed a physically transparent theory of the electronic structure of rare-earth doped silicon, and have computed defect energy levels [299]. This work has laid the foundation for studies of rare-earth doped III-V semiconductors.

j. Adsorption of cobalt on silicon

We have developed a "ring-cluster" model for adsorption of Co on Si. This is one of the first models of metal adsorption in a transition-metal silicide, and is fully consistent with scanning tunneling microscopy observations [289].

k. Defects in large-gap semiconductors

ZnSe, GaN, $A\ell N$, and diamond are but a few of the large-gap semiconductors that offer promise as potential light-emitters/detectors in the visible. We have developed theories relevant to these materials, with an eye toward efficient evaluation of their properties [282,291,302,303].

ℓ. Electronic structure issues

We have developed the theory of semiconductors, especially imperfect semiconductors, is a variety of ways, including studies of deep levels [261,285], the relative importance of (001) and (111) superlattices for efficient luminescence [286], how to probe sub-surface layers with a scanning tunneling microscope [288], the physics of amorphous semiconductors [258], and models of Schottky barriers [251].

4. RECENT PAPERS

241. J. D. Dow, R.-D. Hong, S. Klemm, S. Y. Ren, M.-H. Tsai, O. F. Sankey, and R. V. Kasowski. Proposed explanation of the p-type doping proclivity of ZnTe. Phys. Rev. B

43, 4396-4407 (1991).

250. R. V. Kasowski, M.-H. Tsai, and J. D. Dow. Self-consistent antiferromagnetic ground state for La_2CuO_4 via energy band theory. Phys. Rev. **B 41**, 8949-8954 (1990).

251. R. V. Kasowski, M.-H. Tsai, and J. D. Dow. Formation of Schottky barriers by metal-metal bonds on GaAs. Submitted.

252. S. Y. Ren, W.-M. Hu, G.-L. Yang, and J. D. Dow. Vibrational modes of mass defects in GaP. Submitted.

253. S. Y. Ren, J. Shen, R.-D. Hong, S. Klemm, M.-H. Tsai, and J. D. Dow. Deep levels and shallow-deep transitions in $ZnSe/Zn_{1-x}Mn_xSe$ superlattices. Surf. Sci. **228**, 49-52 (1990).

255. R. V. Kasowski, M.-H. Tsai, J. D. Dow, and M. T. Czyzyk. Self-consistent antiferromagnetic ground state for La_2CuO_4 and CuO via energy band theory. Physica **C 162**, 1349-1350 (1989).

257. S. Y. Ren, W.-M. Hu, and J. D. Dow. Gap vibration modes of mass defects in the cubic compound semiconductor ZnS. J. Lumin. **45**, 159-161 (1990).

258. P. A. Fedders, J. D. Dow, O. F. Sankey, and D. A. Drabold. The role of topology and bond-distortions in determining the character of dopants and band-tailing in a-Si. Submitted

261. J. D. Dow, S. Y. Ren, J. Shen, and M.-H. Tsai. Deep levels in superlattices. In *Impurities, Defects, and Diffusion in Semiconductors: Bulk and Layered Structures,* edited by D. J. Wolford, J. Bernholc, and E. E. Haller, Materials Research Society Symposia Proceedings No. **163**, 349-360 (MRS, Pittsburgh, 1990).

262. O. F. Sankey, D. J. Niklewski, D. A. Drabold, and J. D. Dow. Molecular dynamics determination of electronic and vibrational spectra, and equilibrium structures of small Si clusters. Phys. Rev. **B 41**, 12750-12759 (1990).

263. S. Y. Ren and J. D. Dow. Change of the frontier electronic orbitals due to substitutional impurities in large chemical or biological molecules. Intl. J. Quantum Chem., Quant. Biol. Symp. **17**, 73-80 (1990).

267. S. Y. Ren, W.-M. Hu, G.-L. Yang, and J. D. Dow. Vibrational modes of mass defects in GaP. Proceedings 21st International Conference on the Physics of Semiconductors, Beijing, 10-14 August 1992, edited by Ping Jiang and Hou-Zhi Zheng (World Scientific, Singapore, 1993), pp. 117-120.

270. S. Y. Ren and J. D. Dow. Generalized Möbius transforms for inverse problems. Phys. Lett. **A 154**, 215-216 (1991). Also reprinted in *Some Inverse Problems in Solid State Physics*, ed. Chen Nan-xian, (Beijing University of Science and Technology, Beijing 100083, China, 1992).

271. O. F. Sankey, G. B. Adams, X. Weng, J. D. Dow, Y.-M. Huang, J. C. H. Spence, D. A. Drabold, W.-M. Hu, R.-P. Wang, S. Klemm, and P. A. Fedders. First-principles electronic structure calculations with molecular dynamics made easy. Superlatt. Microstruct. **10**, 407-414 (1991).

272. D. A. Drabold, P. A. Fedders, O. F. Sankey, and J. D. Dow. Molecular-dynamics simulations of amorphous Si. Phys. Rev. **B 42**, 5135-5141 (1990).

276. M.-H. Tsai, O. F. Sankey, and J. D. Dow. Charge transfer in *ab initio* real-space molecular dynamics. Phys. Rev. **B 46**, 10464-10467 (1992).

278. J. Shen, S. Y. Ren, and J. D. Dow. Deep levels in type-II InAs/GaSb superlattices. Phys. Rev. **B 46**, 6938-6946 (1992).

279. J. Shen, S. Y. Ren, and J. D. Dow. Deep-shallow transitions and loss of amphoterism in Type-II superlattices. Phys. Rev. Letters **69**, 1089-1092 (1992).

280. S. Y. Ren, J. D. Dow, and J. Shen. Criteria for Si quantum-well luminescence. J. Appl. Phys. **73** 8458-8462 (1993).

282. D. W. Jenkins, J. D. Dow, and M.-H. Tsai. N vacancies in $A\ell_xGa_{1-x}N$. J. Appl. Phys. **72**, 4130-4133 (1992).

284. J. Shen, J. D. Dow, S. Y. Ren, S. Tehrani, and H. Goronkin. Remote n-type modulation doping of InAs quantum wells by "deep acceptors" in $A\ell$Sb. J. Appl. Phys. **73**, 8313-8318 (1993).

285. S. Y. Ren and J. D. Dow. An improved Lucovsky model of photoionization of deep impurity states in semiconductors. Proceedings 21st International Conference on the Physics of Semiconductors, Beijing, 10-14 August 1992, edited by Ping Jiang and Hou-Zhi Zheng (World Scientific, Singapore, 1993), pp. 1689-1692.

286. S. Y. Ren and J. D. Dow. Comparison of the calculated electronic structures of [111] and [001] $GaAs/A\ell_xGa_{1-x}As$ semiconductor superlattices. Superlatt. Microstruct. **13**, 1-4 (1993).

288. Y. Liang, M.-H. Tsai, W. E. Packard, J. D. Dow, and H. A. Blackstead. Ethereal "interstitials" on the (110) surface of InSb. Solid State Commun. **86**, 33-37 (1993).

289. M.-H. Tsai, J. D. Dow, P. A. Bennett, and D. G. Cahill. Electronic structure and stability of ring-clusters in the Si(111)-($\sqrt{7}\times\sqrt{7}$)Co surface. Phys Rev. **B 48**, 2486-2492 (1993).

291. S. Y. Ren and J. D. Dow. GaN/$A\ell_xGa_{1-x}N$ wurtzite semiconductor superlattices. In Materials Research Society Symposia Proceedings No. **281**, 775-780 (1993).

293. M.-H. Tsai and J. D. Dow. Dimerization on GaN(001) surfaces. In *Materials Theory and Modelling,* edited by J. Broughton, P. Bristowe, and J. Newman, Materials Research Society Symposia Proceedings No. **291**, 309-314 (MRS, Pittsburgh, 1993).

295. H. A. Blackstead and J. D. Dow. Oxide superconductivity. Preprint.

298. J. Shen, S. Tehrani, H. Goronkin, G. Kramer, M. Adam, and J. D. Dow. Semi-insulating, p-type, and n-type doping in $A\ell Sb$, GaSb, and $A\ell Sb$/InAs by a single native defect. Extended Abstracts of the 1993 International Conference on Solid State Devices and Materials, Aug. 29 to Sept. 1, 1993, Nippon Convention Center, Makuhari Messe, Chiba, Japan (The Japan Society of Applied Physics).

299. S. Y. Ren and J. D. Dow. Electronic structure of Si doped by rare-earth Yb^{3+}. In *Rare-earth Doped Semiconductors,* edited by G. S. Pomrenke, P. B. Klein, and D. W. Langer, Materials Research Society Symposia Proceedings No. **301**, 403-408 (MRS, Pittsburgh, 1993).

302. S. Y. Ren, J. D. Dow, and P. A. Fedders. Empirical tight-binding Hamiltonians for diamond and graphite. Submitted.

303. S. Y. Ren and J. D. Dow. Tight-binding sp^3d^5 Hamiltonian for Si. Submitted.

307. J. D. Dow, J. Shen, S. Y. Ren, and W. E. Packard. Deep levels in Type-II superlattices. Mater. Res. Soc. Proceedings, in press.

308. H. A. Blackstead and J. D. Dow. Superconductivity in $YBa_2Cu_3O_x$. Pis'ma Zh. Exp. Teor. Phys. **59**, 262 (1994) [Engl. transl.: Sov. Phys. JETP Lett. **59**, 283 (1994)].

310. H. A. Blackstead, J. D. Dow, and D. B. Pulling. Oxide superconductivity: Integrated, photo-induced high-temperature superconductivity. Submitted.

317. H. A. Blackstead and J. D. Dow. Charge-distributions in $Y_uPr_{1-u}Ba_2Cu_3O_x$. Submitted.

318. H. A. Blackstead and J. D. Dow. Depression of T_c caused by Nd^{+3} pair-breaking in (Rare-earth)$Ba_2Cu_3O_x$. Submitted.

320. H. A. Blackstead and J. D. Dow. Role of Ba-site Pr in quenching superconductivity of $Y_{1-y}Pr_yBa_2Cu_3O_x$ and related materials. Submitted.

321. H. A. Blackstead and J. D. Dow. Implications of Abrikosov-Gor'kov exchange scattering for theories of high-temperature superconductivity. Submitted.

5. PROFESSIONAL PERSONNEL

J. Dow, principal investigator
S. Ren, visiting professor
W. Hu, visiting associate professor
W. Packard, visiting scientist
M. Tsai, assistant faculty fellow
R. Wang, graduate student

6. INTERACTIONS

The principal investigator has functioned as an advisor to the DuPont Corporation on a wide range of topics in materials science, electronics, and solid state physics, and to the Army (Dr. Ruth Nicolaides) on matters related to scanning tunneling microscopy. A new company, Pachyderm Scientific Industries, had been spun-off from the principal investigator's research programs, which manufactures scanning tunneling microscopes for ultra-high vacuum use.

PATENTS

None.

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